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13. ABSTRACT (Maximum 200 words)

A workshop on automatic differentiation of algorithms was held in Breckenridge, Colorado, January 6-9, 1991. This two day workshop was attended by 65 researchers of whom 30 presented half hour lectures and 19 presented posters. Presentations and discussions focussed on (1) theoretical methods and complexity of derivative evaluations and error estimation for composite functions; (2) implementation of the algorithms using precompilers, operator overloading, or other language extensions; and (3) the numerical solution of practical problems with the help of such implementations or hand-coded adjoint equations.

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1991 SIAM WORKSHOP ON AUTOMATIC DIFFERENTIATION OF ALGORITHMS: THEORY, IMPLEMENTATION, AND APPLICATION

Hilton Hotel, Breckenridge, Colorado

January, 6-8.

The workshop was attended by sixty-five researchers, of whom thirty gave half hour lectures, and nine-teen presented posters. This was the first scientific meeting devoted to the topic of automatic differentiation of algorithms. The organizers, Andreas Griewank and George Corliss, were quite successful in their attempt to draw participants from a large variety of fields and institutions. About a third of the participants and speakers came from overseas. The response of the participants was extremely favorable, with many expressing pleasure at the breadth and quality of the work discussed.

As explained by Prof. Masao Iri and Prof. George Cybenko, the *top down* or *reverse* mode of automatic differentiation was already utilized in the early seventies – by Seppo Linnainmaa(1970) for the estimation of rounding errors , and by Paul Werbos for training neural networks by backpropagation. At the same time the forward mode had already been implemented, e.g., in the computer language PROSE, co-authored by Joseph Thames, who presented his integrated applications package at this workshop. Several other speakers presented automatic differentiation implementations, including precompilers for Fortran programs, integrated symbolic/numerical environments for PC's , and implementations by overloading in C++, ADA, and other advanced languages. As an indication of the very strong interest in practical implementations and applications, we note that throughout the workshop it was difficult to gain access to one of the two AT compatibles with modems: the participants were demonstrating their PC software or conducting numerical experiments on their home computers!

The presentations of Prof. Bruce Char and Dr. Victor Goldman were particularly valuable in discussing the relationship between fully symbolic computer algebra and the more numerical technique, which formed the primary focus of this workshop. Both acknowledged that automatic differentiation is significantly more efficient in certain situations and advocated a merging of the two approaches in order to obtain the best of both worlds in terms of flexibility, convenience, and efficiency.

There were many excellent talks on large scale applications – in particular weather modeling, oceanography, petroleum reservoir modeling, beam tracing in optics, satellite orbit analysis, and mechanical systems simulation. Some of the speakers delineated very clearly the remaining deficiencies of currently available automatic differentiation techniques in comparison to handcoded derivative evaluation programs. From the lively discussion that followed, it can be expected that the software developers present will accept the challenge

of closing this gap in efficiency without sacrificing user convenience.

Several speakers pointed beyond the traditional core concern of evaluating point derivatives of first and second order from user-defined programs. They proposed the exploitation of automatic differentiation techniques for the solution of various computational task, e.g., concurrent scheduling on advanced architectures, the numerical solution of differential equations with guaranteed bounds, the efficient calculation of Newton steps, and the parallel solution of unconstrained optimization problems. It became clear that there remain many theoretical and practical challenges, for example, regarding the differentiation of multivariate implicit functions arising in differential algebraic equations.

In many formal and informal discussions, the participants raised the question of how potential users and the scientific community at large can be made aware of the extremely promising computational techniques presented at the workshop. Some felt that the name *Automatic Differentiation* sounds too mechanical and fails to indicate the wealth of intrinsic problems and ramifications. Alas, none of the many alternative suggestion seemed to gain instantly widespread acceptance. The participants did agree on the importance of maintaining the momentum of the woorkshop–for example, by publishing articles in professional news letters and popular scientific journals. The organizers view the publication of well-written and coherent workshop proceedings as a very important first step in popularizing automatic differentiation as a standard computational tool.

The size and format of the workshop appeared fairly optimal. All talks were presented in the same lecture room, with the posters lining the side wall, and one personal computer each placed in the front and back. Despite the unconventional and rather tight schedule, especially on Sunday, the attendance was generally very good, and no more than a handful of attendants left before the final lunch on Tuesday. While only a minority of the attendants used the opportunity to ski in the afternoons, most people seemed to like the setting. The timeslot, early January, was generally considered a good choice, because classes had not yet started or only just begun, so that academics without administrative duties could get away without too much difficulties. However, on account of the low temperatures in the Rockies, early January is not the prime skiing season, and one should be able to secure a better deal from a hotel. The Hilton in Breckenridge had apparently so far little experience with groups like ours, but the friendly staff made every effort to smoothen out minor problems. In particular, they were very accommodating with regards to late cancellations, room changes etc.

Even though many of this year's posters would have warranted an oral presentation, the organizers believe that the automatic diffentiation community is not yet strong enough to support a workshop of comparable quality and originality every year. Therefore we currently consider January 1993 as the earliest appropriate date for the second workshop on the same or a closely related topic. During the intervening time, we will strive to propagate automatic differentiation through minisymposia and short courses at major conferences. Prof. Weldon Lodwick, University of Colorado at Denver, took good care of the computing equipment this time and has offered to assist with all local arrangements should the workshop be held again in Colorado.

Andreas Griewank, George Corliss

Sunday, January 6th, p.m.

1.00 Opening remarks by Andreas Griewank, Argonne National Laboratory

1.15 Prof. Masao Iri, Tokyo University
History of automatic differentiation and error estimation

1.45 Prof. Louis Rall, University of Wisconsin
Point and Interval Differentiation Arithmetics

2.15 Dr. Joseph Thames, Digital Calculus Corporation, CA
A new paradigm in scientific computing

2.45 Prof. George Cybenko, Sirpa Saarinen, and Randy Bramley
CSRD, University of Illinois at Urbana
Neural networks, automatic differentiation, and training algorithms

3.15 - 3.45 Coffee Break

3.45 Prof. John Burns, Virginia Polytechnic
Relation between adjoints and their discretizations

4.15 Dr. Charles Lawson, JPL CalTech
Automatic differentiation of inverse functions

4.45 Introduction of poster presenters and titles

5.00 Prof. Harley Flanders, University of Michigan
Symbolic and Automatic Differentiation of Composite Functions

5.30 Prof. Martin Berz, Michigan State University
Infinitesimals, higher order optical aberrations, and the supercollider

6.15-7.15 Communal Dinner

7.30 Prof. Talagrand, Laboratoire de Meteorologie Dynamique, Paris
The use of adjoint equations in numerical modeling of the atmospheric circulation

8.00 Dr. Piyush Shah, Schlumberger Well Services, Houston
Application of Adjoint Equations to Parameter Estimation in Petroleum Reservoirs and Building Structures

8.30 Dr. W. Thacker, Atlantic Ocean and Meteorological Laboratory, Miami
Solving inverse problems in oceanography using adjoint equations

9.00 Prof. Navon, Florida State University
Derivation and verification of adjoints for a 3D spectral model in meteorology

Monday, January 7th, a.m.

8.00 Dr. Andreas Griewank, Argonne National Laboratory
Automatic Calculation of Jacobians and Newton steps

8.30 Dr. Herbert Fischer and Prof. Klaus Ritter, Technische Universität München
Automatic evaluation of first and second derivatives for optimization

9.00 Prof. Laurence Dixon, Hatfield Polytechnic
The impact of automatic differentiation on (parallel) optimization

9.30-10.00 Coffee Break

10.00 Dr. David Gay, AT&T Bell Laboratories
Differentiation in modeling languages

10.30 Prof. Bruce Char, Drexel University
Computer algebra for program manipulation

11.00 Prof. Victor V. Goldman, J. Molenkamp, and J.A. van Hulzen, University of Twente
Automatic Generation of Efficient Code for Jacobians and Hessians within a Computer Algebra Environment

11.30-5.00 Break

5.00 Mr. Don Layne, Martin Marietta Aeronautics
Application of automatic differentiation and self-validating methods in satellite simulations

5.30 Dr. Rudolf Lohner, Karlsruhe University
Use of symbolic and automatic differentiation in self-validating methods

6.00 Prof. George Corliss, Marquette University
Overloading of point and interval Taylor operators

6.45-7.45 Communal Dinner

8.00 Prof. Leigh Tesfatsion, Iowa State University
Automatic evaluation of higher order partial derivatives for nonlocal sensitivity analysis

8.30 Dr. Leo Michelotti, Fermi National Laboratory
A C++ Implementation of Differential Algebra for Exploratory Orbit Analysis

9.00 Dr. Oscar Garcia, Forest Research Institute, NZ
Automatic differentiation in maximum-likelihood estimation of growth model parameters

Tuesday, January 8th, a.m.

8.00 Prof. Youri Evtushenko, USSR Academy of Sciences
Fast automatic differentiation in optimal control and partial differential equations

8.30 Dr. Vladimir Mazourik, USSR Academy of Sciences
Integration of automatic differentiation into a numerical library for PC's

9.00 Dr. Koichi Kubota, Keio University, Japan
PADRE2, a FORTRAN precompiler yielding error estimates and second derivatives

9.30 Mr. Jim Horwedel, Oak Ridge National Laboratory
Gress, a preprocessor for sensitivity studies on FORTRAN codes

10.00-10.15 Coffee Break

10.15 Dr. Christian Bischof, Argonne National Laboratory
On the road to parallelism in automatic differentiation

10.45 Dr. Edgar Souli, Centre d'Etudes Nuclaires de Saclay
User's experience with FORTRAN precompilers

11.15-12.00 Discussion of software and future developments.

Titles of Posters

1. Y.F. Chang
   A variable-order (10-600) Taylor series method for solving ODE's, with integration steps almost equal to the radii of convergence

2. Bruce Christianson, Hatfield Polytechnic
   Automatic Hessians by reverse accumulation in Ada

3. Robert Corless, University of Western Ontario
   Automatic differentiation in validated defect control for ordinary differential equations

4. Hans Christoph Fischer, University of Karlsruhe
   Differentiation arithmetic and applications in Pascal-XSC

5. William W. Hager, University of Florida
   Dual active sets and constrained optimization

6. David Hill, Temple University and Larry Rich, The Mathematical Software Group
   MATLAB + DERIVATIVES = OPPORTUNITIES

7. James Hu, University of Kansas
   Optimizing computational graphs for automatic differentiation.

8. Baker Kearfott, University of Southwestern Louisiana
   Use of intermediate quantities in expression evaluation to improve the behavior of interval iteration for nonlinear systems

9. Max E. Jerrell, Northern Arizona University
   Automatic Differentiation and Estimation

10. David Juedes, Iowa State University
    ADOL-C, A package for the automatic differentiation of algorithms written in C/C++

11. Thomas Nehrkorn, Atmospheric and Environmental Research, Inc.
    Optimization of model parameters using the adjoint method

12. Richard Neidinger, Davidson College
    Automating arbitrary order derivatives for multivariable functions

13. Dinesh K. Pai, Cornell
    Automatic differentiation in simulation and control of mechanical systems

14. Florian Potra, University of Iowa
    Differentiation of kinematic constraints in multibody dynamics

15. Marcela Rosenblun, Rice University
    Using automatic differentiation in constrained optimization

16. Nicole Rostaing, University of Nice-Sophia Antipolis
    Automatic generation of partial derivatives using REDUCE

17. Herbert Warsitz, Technische Universität München
    Solving constrained and unconstrained non-linear optimization using PADMOS

18. Toshinobu Yoshida, University of Tokyo
    1. ADDS (Automatic Derivative Derivation System)
    2. Why CAN we use second order learning methods for large-scale neural networks?

19. Xaiolei Zou, Florida State University
    Variational 4-dimensional data simulation using an adiabatic version of the NMC spectral model